# 5.5. Semantic utilities for CIF and crystallographic packages

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## 5.5.5. Crystallographic software packages

In spite of the rich semantic content of CIF dictionaries, most crystallographic program packages have been, and will probably continue to be, written with 'static' knowledge of item definitions (see Section [5.1.3. Dictionary usage]). That is, the program authors build in mappings from specific hard-coded data names to components of the internal data structures the software uses in processing data, building models or visualizing structures. This is almost inevitable in software such as refinement programs, where restraints or constraints of arbitrary complexity may be applied at different stages, or where the identification of chemical atom types may change dynamically as the calculation progresses.

Nevertheless, unless a package is designed for use in a quite closed environment, any program that anticipates exchange of input or output data items with other software will benefit from an ability to validate against at least some dictionary attributes.

We present here a brief survey of some of the packages currently in active use within various crystallographic communities, with some comments on their level of support for different elements of the Crystallographic Information Framework. This is of course a snapshot as of mid-2025, and does not claim to be exhaustive.

#### 5.5.5.1. Chemical crystallography

Since the original CIF specification arose from the need to report small-unit-cell organic, inorganic and metal–organic compounds, support for 'traditional' CIFs (using the CIF 1.1 syntax model and with all-underscore data names defined in DDL1 dictionaries) is almost universal in this field. Several packages come with utilities to create CIF output files that satisfy as many conditions for publication as the package can provide.

## 5.5.5.1.1. SHELXL

A dominant refinement program in the field of chemical crystallography, *SHELXL* is one of the *SHELX* family of programs that are also used for structure solution and high-resolution structure refinement of biological macromolecules (Sheldrick, 2008).

The instruction ACTA within a run of *SHELXL* will output two CIF-format files as the basis for a journal submission: 'name.cif' contains experimental metadata, refinement statistics and atom site and geometry information; 'name.fcf' contains the unique set of  $F_{obs}^2, F_{calc}^2$  and  $\sigma(F_{obs}^2)$  values associated with the final refined structure model. The creation of two files is in response to some journals' requirement that structure-factor data be submitted separately from the structural model description.

The .fcf file contains essentially the items in the REFLN category that summarize the squared structure-factor amplitudes of the merged reflections used in the final cycle of refinement, and the refinement statistics reported in the accompanying .cif file are associated with this output. Together, the refinement statistics and .fcf file enable the analysis and validation of the refinement model reported.

To permit independent analysis, SHELXL also outputs unmerged

intensity data. Historically, unmerged data could not be presented in a REFLN table owing to repetition of *hkl* values, although this shortcoming has now been addressed by the introduction of **refln.id** and \_diffrn\_refln.id as category keys. To bypass the historical limitation, unmerged intensities are embedded in the .cif file as a single text field, in the program's native format and labelled \_shelx1\_hk1\_file (Sheldrick, 2015). The refinement instruction set that was used by *SHELXL* is also embedded in the CIF as a text field, also in *SHELXL* native format, labelled \_shelx1\_res\_file.

SHELXL is distributed with an accompanying utility Shred-CIF. This reads a CIF generated by the refinement program, and 'shreds' it into three output files: name.ins, which contains the \_shelxl\_res\_file instruction set, name.hkl, which is the unmerged reflections list, and name\_x.cif, which contains the rest of the information from the original CIF. This machinery allows another SHELXL user to retrieve the original user's modelling environment.

Additional detail of refinement strategies can be provided through the inclusion in the CIF of a *SHELXL* .fab file which accommodates partial structure factors associated with bulk solvent modelling (Spek, 2015; Sheldrick, 2015).

To ensure that the embedded refinement instruction files are a faithful account of the final processing environment of the program, a checksum of the contents of each file is generated and stored alongside their embeddings in the generated CIF (see Table 5.5.5.1).

 Table 5.5.5.1. Local data names used for the encapsulation of SHELXL refinement instructions and reflection data.

Data name	Significance
_shelx_res_file	Refinement instructions
_shelx_res_checksum	Refinement instructions checksum
_shelx_hkl_file	Unmerged reflection data
_shelx_hkl_checksum	Reflection data checksum
_shelx_fab_file	Partial structure factors
_shelx_fab_checksum	Partial structure factors checksum

The *SHELXL* distribution also contains a utility *CIFTAB* that can create pretty-printed tabular output from an input CIF, or that can be used as a templating mechanism to merge site-specific CIF data into a CIF generated by *SHELXL*.

# 5.5.5.1.2. CRYSTALS

*Crystals* (Betteridge *et al.*, 2003) was born in 1975 and developed especially in the early 2000s to make structure determination easier for relatively novice users by providing a powerful graphical user interface and a scripting macro language.

Its interest here is in its development of a small local CIF dictionary to describe refinement of a continuous electron density distribution describable by a particular geometric shape (Schröder *et al.*, 2004). Such an approach has not been widely adopted, but the package authors wanted to record in distributed CIFs the modelling parameters used to associate a special shape with the atom sites possessing such distorted electron densities. Fig. 5.5.5.1 is an example of a description of a disordered group modelled in this way.

loop\_ \_oxford\_atom\_site\_label \_oxford\_atom\_site\_special\_uiso \_oxford\_atom\_site\_special\_size \_oxford\_atom\_site\_special\_declination \_oxford\_atom\_site\_special\_azimuth \_oxford\_atom\_site\_special\_shape F100 0.0894(11) 1.230(3) 1.334(2) 0.320(3) Annulus

Fig. 5.5.5.1. *CRYSTALS* description of a disordered CF<sub>3</sub> group of a CF<sub>3</sub>CO<sub>2</sub>H moiety exhibiting heavy disorder, modelled as an annular-shaped electron density with total occupancy of 3.0 and variable thickness, declination, azimuth and  $U_{iso}$  (Lo *et al.*, 2011). The reserved prefix **\_oxford\_** indicates the provenance of the software developers.

## 5.5.5.1.3. Olex2

*Olex2* (Dolomanov *et al.*, 2009) is probably the current most widespread package for small-molecule crystallography, and extends the *CRYSTALS* paradigm of a graphical-user-interface-driven workflow with macros, Python scripts or extension modules allowing dynamic development.

The package has in-built structure solution and refinement modules, but also supports other programs, such as *SHELXL* for refinement. The need to maintain information pathways between supported modules means that it has wide support for relevant data formats, and for CIF in particular. A CIF metadata module analyses all files in the structure directory, extracting information that can be used to resolve missing items in the final output CIF. It can also make use of the *ShredCIF* facility of *SHELXL* (Section 5.5.5.1.1) to embed or reuse full refinement conditions and reflection data in a CIF.

The native *olex2.refine* module can perform refinements using non-spherical form factors (Dolomanov, 2024) as calculated by *NoSpherA2* (Kleemiss *et al.*, 2021), thereby going considerably beyond the limited extended electron-density capabilities of *Crystals* (Section 5.5.5.1.2) or the multipole refinement approach of *XD2024* (Section 5.5.5.5). There is currently growing interest in the area of quantum crystallography about the possibility of creating CIF dictionary definitions to characterize charge, spin and momentum densities.

## 5.5.5.1.4. PLATON

The program *PLATON* (https://www.platonsoft.nl/platon) was developed in 1980 as a multipurpose crystallographic tool, especially for service crystallography, and has been extended and maintained subsequently to include a large variety of structure analysis and validation components (Spek, 2003; Spek, 2009). Because of its versatility, *PLATON* is used in the IUCr *checkCIF* system to generate validation reports for chemical structures submitted to journals and databases in CIF format (see Section 6.1.4 for more details).

Although *PLATON* does not obtain information dynamically from CIF dictionaries, it has built-in checks for much of the semantic information in the dictionaries (data types, enumeration ranges, valid codes, sensible unit values *etc.*). In addition, it overlays additional constraints on reasonable values of many physical and chemical properties, based on analysis of curated database collections and practitioner experience.

# 5.5.5.2. Support for chemical and macromolecular crystallography

# 5.5.5.2.1. cctbx: a toolbox for chemical and macromolecluar crystallography

The Computational Crystallography toolbox (*cctbx*, Grosse-Kunstleve *et al.*, 2002) was assembled as a library of Open Source tools to provide common functionality for both the chemical and biological macromolecule crystallography communities. It is used in components of other distributed packages such as *Olex2* (Section 5.5.5.1.3) and *PHENIX* (Section 5.5.5.3.2), and is currently maintained as a community GitHub project with over 100 contributors (https://github.com/cctbx/cctbx\_project).

Handling of CIF data is managed by the *iotbx.cif* module (Gildea *et al.*, 2011), which can currently perform validation against the DDL1 core CIF and the DDL2 PDBx/mmCIF dictionary.

## 5.5.5.2.2. GEMMI

*GEMMI* (Wojdyr, 2022) is a cross-platform library, accompanied by a set of small programs, developed primarily for use in the field of macromolecular crystallography (MX). It also supports applications in structural bioinformatics and in chemical crystallography.

The library covers three main areas.

(*a*) It facilitates working with structural models of macromolecules, including reading and writing files in the PDB and mmCIF formats, analysing and modifying models and working with restraint dictionaries (used to restrain geometry of a model from prior knowledge about its component monomers).

(b) It handles crystallographic data, specifically experimentally observed reflections. This includes reading and writing files in the MTZ and mmCIF formats and performing various operations on the reflections.

(c) It also provides tools for working with electron density maps. Such maps can be calculated from both the structural model and experimental data. The library supports reading and writing files in the MRC/CCP4 map format, analysing and modifying the density, and using the fast Fourier transform to switch between direct space and reciprocal space.

In addition to support for PDBx/mmCIF files, *GEMMI* can handle chemical data files described by the DDL1 core CIF dictionary.

#### 5.5.5.3. Macromolecular crystallography

5.5.5.3.1. Collaborative Computational Project Number 4

This project was established in 1979 to support collaborative work in structural biology software development. It created and actively maintains the *CCP4* suite of programs (Agirre *et al.*, 2023) in widespread use worldwide. Interoperability between programs within the *CCP4* suite but also with external programs involves the use of a variety of file formats for specific purposes (*e.g.* its native MTZ reflection data model used in structure refinement), but PDBx/mmCIF files are well supported for data interchange.

Among the ways in which mmCIF is handled by *CCP4* are the following: (*a*) reading and writing of mmCIF files is handled by dedicated libraries, *CCIF* (Keller, 1996) and *MMDB* (Krissinel *et al.*, 2004); (*b*) reflection files in mmCIF format, suitable for deposition of structure factors to the Protein Data Bank, are produced from MTZ files by the program *MTZ2VARIOUS*; (*c*) data harvesting from various of the individual programs involved in the processing pipeline is done through the collation of data items written in mmCIF format, again to facilitate deposition of structure.

tures with the PDB.

Recent versions of *CCP4*, including its cloud implementation (Krissinel *et al.*, 2022), provide a powerful deposition interface developed in collaboration with the Protein Data Bank in Europe that prepares mmCIF files for deposition. It also generates a preliminary wwPDB validation report, allowing users to anticipate the metrics that will be applied to assess the reasonableness of the structural model upon final deposition (Gore *et al.*, 2017).

# 5.5.5.3.2. A Python-based environment for integrated crystallography

*PHENIX* (Adams *et al.*, 2002; Liebschner *et al.*, 2019) is another popular program suite for macromolecular crystallography. Developed partly in response to the structural genomics initiatives of the early 21st century, it is seeking to keep pace with the latest developments in X-ray, neutron and electron crystallography, as well as electron cryo-microscopy.

As with *CCP4*, it handles many internal data formats for specific purposes (such as MTZ for reflection data), but uses mmCIF to import geometry restraints from internal and external ligand libraries. Also as with *CCP4*, it generates PDBx/mmCIF files suitable for deposition of model and structure-factor files, and can interact with the wwPDB OneDep system to generate validation reports (see Section 7.2.3.1).

#### 5.5.5.3.3. Visualization of protein structures

Several visualization tools exist that can import PDBx/mmCIF files. Their success demonstrates their ability to interpret structural information about protein and nucleic-acid macromolecules and their ligand environments. Among the most widespread are (in alphabetical order): *CCP4mg*, a molecular-graphics program within the *CCP4* (Section 5.5.5.3.1) suite, *ChimeraX* (Meng *et al.*, 2023), *COOT* (Emsley *et al.*, 2010), *iCn3D* (Wang *et al.*, 2019), *Jmol/JSmol* (Hanson, 2004 onwards, and see Section 5.6.5), *PyMOL* (Schrödinger LLC, 2015).

#### 5.5.5.4. Powder diffraction

The powder diffraction CIF (pdCIF) standard has been adopted more gradually within its user community than the single-crystal version. This may be in part because of the typically more complex results of a powder structure analysis, where several phases are present, or where several data sets are collected for studying the variation of physical properties with temperature, pressure or other environmental conditions. The multiblock CIF dictionary (Chapter 3.3) is intended in part to address the need to correlate data blocks in such multi-parameter studies.

A contemporary review of the use of CIF in powder diffraction was published by Toby (2019).

#### 5.5.5.4.1. GSAS-II

*GSAS-II* was developed as 'a general purpose package for data reduction, structure solution and structure refinement that can be used with both single-crystal and powder diffraction data from both neutron and X-ray sources, including laboratory and synchrotron sources, collected on both two- and one-dimensional detectors' (Toby & Von Dreele, 2013).

For complex powder diffraction studies, it has a sophisticated user interface that allows the user to construct a single CIF containing separate datablocks for each phase identified and for each measured data set. Template files are included with the software that allow easy reuse of persistent information such as instrument characteristics that are relevant to each portion of the CIF to be generated. The relationship between the information in each data block is managed through the use of block pointers \_pd\_block.id and \_pd\_block\_diffractogram.id (Section 3.6.8.1). This approach is now formally deprecated because the multiblock protocol described in Chapter 3.3 is more general and extensible. Nevertheless, a significant number of archived files that use the older mechanism exist.

An earlier iteration of this program did not have native pdCIF support, but could also produce CIFs with the same organizational structure through the use of a helper program, *GSAS2CIF* (Toby *et al.*, 2003).

# 5.5.5.4.2. TOPAS

Another software suite widely used for Rietveld refinement, *TOPAS* (Coelho, 2018), does not have native pdCIF support but can produce structured pdCIF output by means of a series of independently developed macros (Rowles, 2022).

#### 5.5.5.4.3. Visualization tools for powder CIF

A small number of programs exist that can read pdCIF input files and display powder profiles. The IUCr web program *plotCIF* (Westrip & Toby, 2013), based on an earlier program *pdCIFplot* (Toby, 2003), can read any small-molecule CIF file and display observed or computed powder diffraction patterns. Where experimental powder data are present in the CIF the profile and difference plots can be displayed, zoomed and plotted as desired on  $2\theta$ , Q or *d*-spacing axes. If there is no powder data (for example in a single-crystal structure determination), the application can call the program *PLATON* (Section 5.5.5.1.4) to generated a simulated powder pattern.

*pdCIFplotter* (Rowles, 2022) is a standalone Python program that provides similar functionality, but can simultaneously display multiple diffraction patterns using either a stack plot to separate each pattern by a vertical offset, or a surface plot where the intensity of each point is represented by a colour.

IUCr journals request and disseminate Rietveld profiles and other experimental data sets in CIF format, thus providing a ready source of pdCIF input files for use by such programs.

#### 5.5.5.5. Support for electron density modelling

Description of extended (non-sperical) electron density distribution is currently supported by CIF through data names defined in the rhoCIF dictionary (Chapters 3.8 and 4.8). This makes use of an atom-centred multipole expansion model (Stewart, 1973; Hansen & Coppens, 1978) that was developed computationally by the program *XD* (Koritsanszky *et al.*, 2003). The latest version of this software, *XD2024* (Volkov *et al.*, 2016), retains full support for rhoCIF.

Multipole coefficients in CIF format are output by other software that uses the Hansen–Coppens formalism, such as *MoPro* (Jelsch *et al.*, 2005) and *JANA2020* (Petříček *et al.*, 2023).

#### 5.5.5.6. Topology

Topological nets are a comparatively recent introduction to mainstream crystallography, and the reference implementation for the topology CIF dictionary (Chapters 3.10 and 4.10) is *ToposPro* (Blatov *et al.*, 2014). The visualization program *Jmol/JSmol* (Hanson, 2004 onwards) can also read and render the nets specified in the topoCIF format.

### 5.5.5.7. Support for modulated and magnetic structures

As structure determination techniques continue to evolve and more complex structural features are of interest, especially to materials scientists, novel CIF dictionaries to describe particular fields of interest begin increasingly to overlap. Programs such as JANA2020 (Petříček et al., 2023) are increasingly able to analyse and describe commensurate and incommensurate modulated structures, complex twinning, and to handle multiphase materials and dynamically refined microstructure. The need to articulate novel concepts and encapsulate them in standard data interchange protocols is encouraging active software development in step with the development of new CIF dictionaries. Jmol/JSmol (Hanson, 2004 onwards) is another application that can handle a growing number of novel structural representations, and its ability to provide powerful visualizations of new properties (see Section 5.6.5 for some examples) makes it a synergistic research tool across these new developments.

Among programs used for the determination or refinement of magnetic structures are JANA2020, GSAS-II (Toby & Von Dreele, 2013), FullProf (RodrAguez-Carvajal, 1993) and TOPAS (Coelho, 2018).

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## 5.5. SEMANTIC UTILITIES FOR CIF AND CRYSTALLOGRAPHIC PACKAGES

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